# A Landauer transport formulation with inelastic scattering

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The Landauer transport formulation is generalized to the case of a dynamic scatterer with an arbitrary energy level structure, weakly coupled to a long ideal noninteracting wire. The two-terminal *linear* conductance of the device is expressed in terms of the (in general inelastic) scattering cross sections of the electrons off the scatterer, using a Fermi-liquid picture for the scattering states of the whole system. Assuming unitarity, i.e. the optical theorem, we obtain the same results from a Kubo linear response treatment and from a Keldysh technique approach.

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**Introduction.** The scattering model due to Landauer [1] has been extremely useful for studies of the electronic transport in mesoscopic systems, since it gives a clear physical picture of the processes involved (for reviews, see Refs. 2 and 3). This formulation expresses the linear conductance $\mathcal{G}$ of a given finite sample (the scatterer) in terms of transmission probabilities for electrons injected to and collected from it, via ideally conducting leads. For noninteracting electrons, with a total transmission amplitude $t$ and magnitude $\mathcal{T} = |t|^2$, the two-terminal single-channel Landauer formula, including spin, reads

$$\mathcal{G} = \frac{2e^2}{h}\mathcal{T}. \tag{1}$$

In this paper we generalize his result to include inelastic scattering by the sample.

A general formal expression for the conductance of a scatterer imbedded in a long, ideal, "wire" was given in Ref. 4. It was proven to reduce to the Landauer formula (1) at the zero temperature ($T \to 0$) limit. However, at finite $T$ it was not possible to produce such a proof, and the inelastic scattering channels, which open up then, were implicated. Later, the opinion that the Landauer formula is not applicable with interactions on the scatterer became prevalent (e.g. Ref. 5). That would mean that many of the usual mesoscopic effects would be severely modified by the inelastic scattering and interactions. Thus, the generalization (see also Ref. 6) we propose is relevant. Indeed, the *full* scattering matrix of a local perturbation in an otherwise ideal conducting wire, should contain the necessary physical information for the conductance. The quasiparticle picture is necessary to approximately include the effects of electron-electron interactions on the leads mediated by virtual second-order processes on the scatterer. Within this picture, multiparticle processes and non-Fermi-liquid behavior are avoided.

The linear dc conductance of the sample, at finite temperatures, is simply expressed through its full single-quasiparticle scattering matrix (satisfying unitarity and time-reversal symmetries). The results are then confirmed via the Kubo linear response approach [7], considering the sample as a set of scattering states with equilibrium populations. Finally, we use the optical theorem [8] to express the linear Keldysh [4, 9, 10, 11] conductance in terms of the sample's transmission cross-sections, also confirming the generalized Landauer result.

**Scattering formulation for a one-dimensional (1D) conductor.** We demonstrate our statement for the simple case of a scatterer (a "quantum dot"), taken as a *finite* "black box" with *arbitrary interactions inside it*, coupled weakly to ideal 1D leads. We start by writing the scattering states, including inelastic processes. The states coming from the left ($\ell$) and from the right ($r$) belong to two independent Hilbert spaces, with no mutual Fermi blocking factors. For linear transport, the two chemical potentials of the ($\ell$) and ($r$) states, $\mu_\ell$ and $\mu_r$ respectively, are slightly different ($\mu_r < \mu_\ell$, $\mu_\ell - \mu_r \equiv eV << \mu_{\ell,r}$). At equilibrium, both spaces are populated with the same temperature $T$ and $\mu_\ell = \mu_r = \mu$. Without the coupling, the states $|i\rangle$ of the dot have discrete energy levels, $\epsilon_i$, including the arbitrary interactions there. The leads have continuous spectra, characterized by a wavenumber $k$, longitudinal velocity $v \equiv \hbar k/m$ and a kinetic energy of the "incoming" electron $E \equiv \hbar^2 k^2/2m$. The states coming from the left lead (labelled by $\ell$) are

$$\begin{aligned} \mid \ell k i\rangle = e^{ikx} \mid i\rangle + \sum_j r_{ji}\sqrt{\frac{v}{v_j}}\, e^{-ik_j x} \mid j\rangle, \\ \text{and} \quad \sum_j t_{ji}\sqrt{\frac{v}{v_j}}\, e^{ik_j x} \mid j\rangle, \end{aligned} \tag{2}$$

far to the left of the dot and far on its right, $v_j = \hbar k_j/m$ ($> 0$) is defined by $\hbar^2 k_j^2/2m \equiv E - \epsilon_j + \epsilon_i$, $t_{ji}$ and $r_{ji}$ are the transmission and reflection amplitudes from the left, exciting the dot from state $|i\rangle$ to state $|j\rangle$. The

states coming from the right lead are

$$| rki\rangle = \sum_j t'_{ji}\sqrt{\frac{v}{v_j}}\, e^{-ik_j x} \mid j\rangle, \quad \text{and}$$
$$e^{-ikx} \mid i\rangle + \sum_j r'_{ji}\sqrt{\frac{v}{v_j}}\, e^{ik_j x} \mid j\rangle, \tag{3}$$

far to the left of the scatterer and far on its right, with the transmission and reflection amplitudes $t'_{ji}$ and $r'_{ji}$. Using $\mathcal{T}_{ij} \equiv |t_{ij}|^2$, $\mathcal{T}'_{ij} \equiv |t'_{ij}|^2$, $\mathcal{R}_{ij} \equiv |r_{ij}|^2$, $\mathcal{R}'_{ij} \equiv |r'_{ij}|^2$, the total right-going current in the states (2) with an energy $E$ in a window $dE$, per spin direction, is

$$I_{\ell ki} = ev \sum_j \mathcal{T}_{ji} n_i dE = \frac{e}{2\pi\hbar} \sum_j \mathcal{T}_{ji} dE, \tag{4}$$

where $n_i = (2\pi\hbar v)^{-1}$ is the density of $\{\ell ki\}$ states per spin channel (which cancels the velocity factor, as usual).

We next discuss the thermal occupations. The probability to find the dot in state $|i\rangle$ is $P_i$, with $\sum_i P_i = 1$. Consider a typical low-lying excited state of the whole system with the dot in state $|i\rangle$. Within a Fermi liquid description the number of quasiparticles in this state is macroscopic. Thus the contribution of the dot energy $\epsilon_i$ to the energy of a single quasiparticle state is negligible. Hence their populations are given by the Fermi function *of the electronic energy only*. Thus, the populations of the scattering states $| \ell ki\rangle$ and $| rki\rangle$ are

$$P_{\ell ki, rki} = P_i f(E - \mu_{\ell,r}), \tag{5}$$

where $f(x) = 1/(e^{\beta x} + 1)$ is the Fermi function and $\beta = (k_B T)^{-1}$. The total populations of incoming electrons with energy $E$ are given by $f_{\ell,r}(E) = f(E - \mu_{\ell,r})$.

The averaged right (left)-going current carried by the $\ell$ ($r$) states is given by

$$\begin{aligned} I_{\ell\to r} &= \sum_i P_{\ell ki} I_{\ell ki} = \frac{e}{2\pi\hbar}\int dE \sum_{ij} P_{\ell ki} T_{ji}; \\ I_{r\to\ell} &= \frac{e}{2\pi\hbar}\int dE \sum_{ij} P_{rki} \mathcal{T}'_{ji}. \end{aligned} \tag{6}$$

For a finite, time-reversal symmetric dot, with real eigenstates, $\mathcal{T}_{ji} = \mathcal{T}'_{ji}$, meaning that the cross-section for scattering of an electron from the dot, flipping the dot from state $i$ to state $j$, has the same value irrespective of the direction from which the electron is coming. The total average net current is given by $I = I_{\ell\to r} - I_{r\to\ell}$. Using Eq. (5), we find, to first order in $eV \equiv \mu_\ell - \mu_r$, that the linear conductance, $\mathcal{G} \equiv \lim_{V\to 0} I/V$ per spin is

$$\mathcal{G} = \frac{e^2}{2\pi\hbar}\int dE \Big(-\frac{\partial f}{\partial E}\Big)_\mu \sum_{ij} P_i \mathcal{T}_{ji}. \tag{7}$$

This is the two-terminal single-channel, finite-$T$ Landauer linear conductance formula including arbitrary interactions on the scatterer and inelastic scattering.

**Rederivation from the Kubo formula.** Here, we confirm our main result, Eq. (7), using the $\omega \to 0$ limit of the Kubo linear response formulation [7],

$$\mathcal{G}(\omega) = \frac{\pi e^2}{\omega}[S_v(-\omega) - S_v(\omega)]. \tag{8}$$

The velocity power spectrum, $S_v(\omega)$ is given for Fermi liquid electrons in a unit volume and including spin by

$$S_v(\omega) \equiv \sum_{m,n} |\hat{v}_{mn}|^2 \delta(\hbar\omega - E_m + E_n) \times P_i f(E_m - \mu)[1 - f(E_n - \mu)]\,, \tag{9}$$

where the matrix elements of the velocity operator $\hat{v}$ (in the wire direction) are taken between an initial state $|m\rangle = |\ell ki\rangle$, or $|rki\rangle$ and a final one, $|n\rangle = |\ell k'i'\rangle$, or $|rk'i'\rangle$. $k$ is related to $E = E_m$ and $k'$ to $E' = E_n$. The summation over $m$ means summation over $i$, taking the sum of the $\ell$ and the $r$ terms and integrating over the energy $E$ (which, as explained above, does not contain the dot energy), with the appropriate density of states, and similarly for the summation over $n$. Note that here the Fermi blocking factors, $[1 - f(E_n - \mu)]$, *do* appear, since *real transitions* are considered. The conductance is proportional to the *net* absorption rate from a classical field at frequency $\omega$ [12].

The transitions are of four types: $(\ell,\ell)$ (left-moving to left-moving), $(\ell, r)$ (right-moving to left-moving), and similarly $(r, r)$ and $(r, \ell)$. The sum of the two latter transitions equals that for the two former ones, so we calculate only the former, and multiply the final result by two. From Eq. (2),

$$\begin{aligned} \langle \ell ki|\hat{v}|\ell k'i'\rangle &= \frac{\sqrt{vv'}}{2}\sum_j (t^*_{ji}t_{ji'} + \delta_{i,i'} - r^*_{ji}r_{ji'}) \\ &= \sqrt{vv'}\sum_j t^*_{ji}t_{ji'}, \end{aligned} \tag{10}$$

where $v' = \hbar k'/m$ and we used the (column) unitarity properties of the full S-matrix, $\sum_j t^*_{ji}t_{ji'} = \delta_{i,i'} - \sum_j r^*_{ji}r_{ji'}$. Likewise, $\langle \ell ki|\hat{v}|rk'i'\rangle = \sqrt{vv'}\sum_j t^*_{ji}r'_{ji'}$. Taking the absolute values squared of these matrix elements, summing over $i'$, (together with the density-of-states factors required to convert the $k$- and $k'$-sums into energy integrals) and using the (row) unitarity properties of the full S-matrix, $\sum_{i'}(t^*_{ji'}t_{j'i'} + r'^*_{ji'}r'_{j'i'}) = \delta_{j,j'}$, yields

$$\sum_{i'} n_i n_{i'} \big(|\langle \ell ki|\hat{v}|\ell k'i'\rangle|^2 + |\langle \ell ki|\hat{v}|rk'i'\rangle|^2\big) = \frac{1}{h^2}\sum_j \mathcal{T}_{ji}. \tag{11}$$

Adding a similar contribution from the states which start in $|rki\rangle$, we put the resulting expression into Eq. (9), and use $f(E + \hbar\omega/2)[1 - f(E - \hbar\omega/2)] = f(E)[1 - f(E)] + (\hbar\omega/2)f'(E) + \mathcal{O}(\omega^2)$, to obtain for small $\omega$,

$$S_v(\omega) = \frac{2}{h^2}\int dE\big[f(1-f) + (\hbar\omega/2)\Big(\frac{\partial f}{\partial E}\Big)\big]\sum_{ij} P_i \mathcal{T}_{ji}.$$

Eq. (8) now yields Eq. (7) for $\mathcal{G}(\omega=0)$, as required.

**Confirmation via the Keldysh technique.** It has been claimed [4, 5] that when the transmitted electron is subject to inelastic interactions on the scatterer, the transmitted current should be obtained using methods applicable to many-body problems. The most-frequently used one is the Keldysh technique. Here we calculate independently the transmission of the system from the full scattering operator, and the current using the Keldysh technique, and then confirm that the two expressions so obtained are identical. Moreover, this equivalence is just a result of the *optical theorem*, namely, it follows from the assumed unitarity of the *full* scattering matrix.

Considering a quantum dot with a single electronic level, the coupling with the leads is $\sum_k V_{\ell k} c^\dagger_{\ell k} d + \sum_p V_{rp} c^\dagger_{rp} d + hc$. (The band states on the left are denoted by the wavevector $k$ and those on the right by $p$. Both leads are identical, except of being connected to reservoirs of different chemical potentials. $d^\dagger$ creates an electron on the dot.) The current between the leads is given by the one flowing from the left, $I_\ell = e(d/dt)\sum_k \langle c^\dagger_{\ell k} c_{\ell k}\rangle$ (where $\langle ...\rangle$ is the quantum average), or by its counterpart $-I_r$. In the Keldysh technique these currents are expressed in terms of various Green functions, resulting in (see, e.g., Ref. 9)

$$I = \frac{e}{\hbar}\int d\omega \Big(f_\ell - f_r\Big)\Big[\frac{i}{\pi}\frac{\Gamma_\ell\Gamma_r}{\Gamma_\ell+\Gamma_r}\Big(\overline{G^R_d} - \overline{G^A_d}\Big)\Big], \quad (12)$$

where the partial widths,

$$\Gamma_{\ell,r}(\omega) \;=\; \pi\sum_k |V_{\ell k,rp}|^2 \delta(\hbar\omega - \epsilon_{k,p}), \quad (13)$$

are needed only in a narrow energy interval around the (average) Fermi level of the leads. Therefore, one may neglect the energy-dependence of these widths [8]. $\overline{G^{R,A}_d}(\omega)$ are the thermal averages of the usual retarded and advanced Green functions on the dot, which include all interactions. Despite the apparent similarity of Eq. (12) to the Landauer formula, it has been claimed [9] that there is no connection between the terms in the square brackets there and the transmission, once inelastic scattering is present. However, as we show below, these terms are in fact identical to the transmission.

The transmission is derived from the full scattering operator of the system, $S$. Writing the total Hamiltonian of the system as $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, where $\mathcal{H}_0$ is the Hamiltonian of the disconnected system (including the interactions on the dot) and $\mathcal{H}_1$ describes the coupling between the dot and the leads, then (to all orders in $\mathcal{H}_1$), $S = \lim_{t\to\infty} U(t)$, where

$$U(t) = 1 - \frac{i}{\hbar}\int_{-\infty}^{t} dt' e^{i\frac{\mathcal{H}_0}{\hbar}t'}\mathcal{H}_1 e^{-i\frac{\mathcal{H}_0}{\hbar}t'} - \int_{-\infty}^{t}\frac{dt'}{\hbar}\int_{-\infty}^{t'}\frac{dt''}{\hbar} e^{i\frac{\mathcal{H}_0}{\hbar}t'}\mathcal{H}_1 e^{-i\frac{\mathcal{H}}{\hbar}(t'-t'')}\mathcal{H}_1 e^{-i\frac{\mathcal{H}_0}{\hbar}t''}. \quad (14)$$

The transition probability per unit time between two states of the system, $|m\rangle$ and $|n\rangle$, is given by

$$W_{m\to n} = \lim_{t\to\infty}\Big(\langle m|U^\dagger|n\rangle\frac{d}{dt}\langle n|U|m\rangle + cc\Big). \quad (15)$$

When one specifies to the case in which both states $|m\rangle$ and $|n\rangle$ have no electron on the dot and differ only by one electron being on the left lead in the former and on the right lead in the latter, one finds [8, 10]

$$W_{k\to p} = \frac{|V_{\ell k}V_{rp}|^2}{\hbar^4}\int_0^\infty d\tau_1 d\tau_2 d\tau_3 e^{i\frac{\epsilon_k(\tau_3-\tau_1)}{\hbar}} e^{i\frac{(\epsilon_p-\epsilon_k)\tau_2}{\hbar}} \times G^A_d(-\tau_2-\tau_1,-\tau_2)G^R_d(0,-\tau_3) + cc. \quad (16)$$

The Green functions appearing here depend on two time arguments (and not on their difference alone), since the thermodynamic average has not yet been performed. It is of crucial importance to realize that the Green functions appearing in the Keldysh technique result (12) for the (linear response) current are the Fourier transform of the *thermodynamically averaged* Green functions. On the other hand, the transition probability per unit time includes a product of *two* Green functions. Obviously, the thermodynamic average of the product is not necessarily the product of the two averages. The relation between the two is supplied by the optical theorem.

The transmission from a state of an electron with energy $E = \hbar\omega$ on the left lead to a state of an electron with energy $E' = \hbar\omega'$ on the right lead is [8] $\mathcal{T}(\omega\to\omega') = \sum_{k,p}\overline{W}_{k\to p}\delta(\frac{\epsilon_k}{\hbar}-\omega)\delta(\frac{\epsilon_p}{\hbar}-\omega')$. Hence, the total transmission probability of an electron having initial energy $\hbar\omega$ is $\mathcal{T}(\omega) = \int d\omega'\mathcal{T}(\omega\to\omega')$. For overall energies near $\mu$, $\mathcal{T}(\omega)$ is identical to the quantity $\sum_{ij}P_i\mathcal{T}_{ji}$ which appeared in Eq. (6). With the definitions (13), $\mathcal{T}(\omega)$ becomes

$$\mathcal{T}(\omega) \;=\; \frac{2\Gamma_\ell\Gamma_r}{\hbar^2\pi}\int_0^\infty d\tau_1 d\tau_2 e^{i\omega(\tau_2-\tau_1)} \times\overline{G^A_d(-\tau_1,0)G^R_d(0,-\tau_2)}, \quad (17)$$

and consequently, using the Landauer formulation (see also Ref. 11)

$$I = e\int d\omega\Big(f_\ell(\omega) - f_r(\omega)\Big)\mathcal{T}(\omega). \quad (18)$$

Next we show that the two expressions, Eqs. (12) and (18), are identical, namely, that the terms in the square brackets in Eq. (12) are given by $\mathcal{T}(\omega)$, Eq. (17). To this end, we use Eq. (14) to write down explicitly the condition that $S$ is unitary, $\sum_m\langle n|S^\dagger|m\rangle\langle m|S|l\rangle = \delta_{n,l}$. Specifying to the case in which the states $|l\rangle$ and $|n\rangle$ differ just by one electron taken from the left to the right lead, the unitarity condition becomes

$$0 = \frac{V^*_{\ell k}V_{rp}}{\hbar^4}\int_{-\infty}^{\infty} dt' dt'' e^{i(\frac{\epsilon_p}{\hbar}t' - \frac{\epsilon_k}{\hbar}t'')}\Big[i\Big(G^A_d(t',t'')$$

$$- \; G_d^R(t',t'')\Big) + \int_{-\infty}^{\infty} dt_1 dt_2 G_d^A(t',t_1) G_d^R(t_2,t'') \times\Big(\sum_{p'} |V_{rp'}|^2 e^{i\frac{\epsilon_{p'}(t_2-t_1)}{\hbar}} + \sum_{k'} |V_{\ell k'}|^2 e^{i\frac{\epsilon_{k'}(t_2-t_1)}{\hbar}}\Big)\Big]. \tag{19}$$

Since $\Gamma_{\ell,r}$ are independent of the energy, we have $\sum_{k,p} |V_{\ell k,rp}|^2 e^{i\frac{\epsilon_{k,p}}{\hbar}t} = 2\Gamma_{\ell,r}\delta(t)$. Performing the thermodynamic average over Eq. (19), taking into account that $G^R(t_1,t_2)$ $(G^A(t_1,t_2))$ is defined for $t_1 \geq t_2$ $(t_1 \leq t_2)$, and that $\overline{G^{R,A}(t_1,t_2)}$ depends only on $(t_1-t_2)$, we find

$$- \; iV_{\ell k}^* V_{rp}\Big[2\pi\delta(\epsilon_k-\epsilon_p)\Big(\overline{G_d^R(\epsilon_k)} - \overline{G_d^A(\epsilon_k)}\Big) + \; 2i\frac{\Gamma_\ell+\Gamma_r}{\hbar^2}\int_{-\infty}^{\infty} dt e^{i\frac{(\epsilon_p-\epsilon_k)t}{\hbar}} \int_0^{\infty} d\tau_1 d\tau_2 e^{i\frac{\epsilon_k(\tau_2-\tau_1)}{\hbar}} \times\overline{G_d^A(t-\tau_1,t)G_d^R(t,t-\tau_2)}\Big] = 0. \tag{20}$$

Since the thermal average in the second term here is independent of $t$, the $t-$integration yields $2\pi\delta(\epsilon_k-\epsilon_p)$ and Eq. (20) gives

$$\overline{G_d^R(\epsilon_k)} - \overline{G_d^A(\epsilon_k)} = -i\pi\frac{\Gamma_\ell+\Gamma_r}{\Gamma_\ell\Gamma_r}\mathcal{T}(\epsilon_k), \tag{21}$$

which shows that the square brackets in Eq. (12) are equal to $\mathcal{T}(\omega)$, Eq. (17). That is, the current using the Keldysh method, Eq. (12), and the same current by the Landauer-type formula, Eq. (18), are identical. We have confirmed this equivalence explicitly by considering the case in which the electrons on the dot interact with a phonon bath [13].

**Conclusions.** Within the Landau framework (used here for single-quasiparticle scattering states), we found that the Landauer-type picture for the *linear* transport is generalizable to include *inelastic* scattering and interactions on the "dot". We considered here a dot having, when it is closed, an arbitrary energy level structure, due to (possibly strongly interacting) degrees of freedom (e.g. vibrations, spins) *other* than those of the conduction electrons. The results were confirmed with both the linear response and Keldysh approaches. Unitarity and time-reversal symmetries for the dot played crucial roles. However, the generalization for a dot imbedded in an Aharonov-Bohm interferometer is straightforward. So are those to multichannel and multiterminal situations.

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